Pump and probe experiments from first principles

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The development of ultra-short laser pulses has opened the opportunity to investigate the dynamics of electrons on the femto-second time-scale (1 fs=1.E-15 seconds). After the photo-excitation with such lasers pulses, electrons are in a regime which is highly out-of-equilibrium and a great variety of physical processes can be exploited. The theoretical modelling of such processes is very challenging. First principles approaches offer a natural solution, but the description of non-equilibrium physics from first principles is computationally very demanding.

Here I present a novel numerical approach, based on the merging of the out-of-equilibrium Green's function method with the ab-initio, Density-Functional-Theory, to describe this regime in semi-conductors. [1-5] Silicon [6-7] is used as reference material. Moreover, I consider MoS2 [8] and WSe2 [9] monolayers and discuss transient absorption and transient Kerr in these systems. In both cases the simulations are compared with recent measurements.

Finally, a general comparison of the computational requirments with more common first principles simulations is considered.
I forsee that the development of HPC centers and advanced computational facilities will have key importance for the development and spreading of computational studies describing non-equilibrium physics.

REFERENCES:

[1] C. Attaccalite, M. Gruning, A. Marini, Phys. Rev. B 84, 245110 (2011)
[2] A. Marini, J. of Phys: Conf. Ser. 427, 012003 (2013)
[3] D. Sangalli and A. Marini, J. of Phys: Conf. Ser. 609, 012006 (2015)
[4] E. Perfetto, D. Sangalli, A. Marini, G. Stefanucci, Phys. Rev. B 92, 205304 (2015)
[5] E. Perfetto, D. Sangalli, A. Marini, G. Stefanucci, Phys. Rev. B 94, 245303 (2016)
[6] D. Sangalli, and A. Marini, Europhysics Letters 110, 47004 (2015)
[7] D. Sangalli, S. Dal Conte, C. Manzoni, G. Cerullo and A. Marini, Phys. Rev B 93, 195205 (2016)
[8] E. Pogna, M. Marsili, D. De Fazio, S. Dal Conte, C. Manzoni, D. Sangalli,
D. Yoon, A. Lombardo, A. Ferrari, A. Marini, G. Cerullo, D. Prezzi, ACS nano 10, 1182 (2016)
[9] A. Molina Sanchez, D. Sangalli, L. Wirtz, and A. Marini, Nano Letters 17, 4549 (2017)